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ABSTRACT: A theoretical investigation of the propagation of a detonation wave is made. The problem of the occurrence of detonation in a nonuniformly heated gas capable of a chemical reaction is solved numerically. The three reaction flow conditions possible are developed.

Gas detonation waves usually are investigated in pipes, and the detonation is initiated by a shock wave, or by an accelerating flame. The initial temperature of the combustible mixture is close to ambient. The fact of the formation of a detonation wave in these experiments can be readily established by the rapid change in pressure, or temperature. As is known, the rate at which the chemical change takes place in the detonation mode is accelerated many times. /76*

The situation is different during the operation of an internal combustion engine, when so-called "knocking" takes place. Because of the preliminary compression of the combustible gas, and its mixing with the products of combustion remaining from the preceding cycle, the temperature of the gas in the cylinder can become so high that conditions become favorable for an explosive-like volumetric flow of the chemical reaction. If temperature conditions, and the conditions under which the mixing occurs are identical throughout the cylinder volume, the chemical reaction causes a uniform rise in pressure throughout the volume. But if the temperature of the combustible mixture is different at different points in the volume, the reaction at these points will not be identical, and nonuniform expansion of the gas will result. The consequence is possible formation of shock and detonation waves.

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* Numbers in the margin indicated pagination in the foreign text.

As distinguished from classic investigations of detonations in pipes, the recording of the transition from a condition in which the explosive-like flow is uniform to one of a propagating detonation wave is a difficult experimental task, and requires precise measurements.

This paper is devoted to a theoretical investigation of this question. The problem of the occurrence of detonation in a nonuniformly heated gas capable of a chemical reaction is solved numerically. It is shown that three reaction flow conditions are possible. If the temperature distribution specified at the initial moment in time is such that the gas is heated almost uniformly, the reaction will take place in the thermal explosion mode. When the initial temperature profile is very steep, a shock wave occurs and breaks away from the reaction wave. Finally, there exists that distribution of temperature such that the forming shock wave is capable of causing a reaction, and a steady-state detonation mode occurs.

1. Statement of the problem. Let there be given a temperature profile for a gas capable of reacting and filling a half-space $X > 0$, in the form of the following linear function at the initial moment in time

$$T(0, X) = T_0 - \varkappa X \tag{1.1}$$

Moreover, gas pressure, P, and the relative concentration of the combustible component, a, are constants, while the gas is at rest, that is

$$P(0, X) = P_0, \quad U(0, X) = 0, \quad a(0, X) = 1 \tag{1.2}$$

where $U(t, X)$ is the gas velocity.

In order to satisfy the condition $T(t, X) \geq 0$ $(0 \leq t \leq \infty)$, we will say that $T(0, X) = 0$ when $X > T_0/\varkappa$. If only the initial stage of development of the disturbances is of interest (and this is sufficient, as we will see from what follows), the latter requirement is not restrictive because of the finiteness of the rate at which the disturbances are propagated.

The gas will be assumed perfect; that is, the equation of state is in the form

$$PV = RT \tag{1.3}$$

Here R is the gas constant, and V is the specific volume for the gas.

From the way in which the problem is stated, we see that the specified original state is steady for a perfect, non-reacting gas. Accordingly, the gas will change its original state only because of the initiating chemical reaction. Gas motion within the vessel should occur. Since the reaction will develop with greater intensity at the hot wall, the gas will expand at that wall, and the formation of a shock wave is possible. Given predetermined conditions, this wave can become a detonation wave. /77

There are various conditions possible for the course of the chemical reaction, depending on the original, specified, temperature gradient.

In the case of large $\varkappa$, the forming shock wave will be weak because the characteristic time for the development of the chemical reaction increases sharply with distance from the hot wall, and by the time the reaction reaches that wall the shock wave has long since escaped from the wall.

In the case of a reduction in $\varkappa$, the induction time is reduced, and the gas layers further away from the hot wall begin to play a role in the formation of the shock wave. The shock wave gets stronger, the result of the energy release in these layers. It should be expected that there are also $\varkappa$ at which the intensity of the shock wave will be sufficient to initiate a reaction in the gas. In such case the reaction will occur in the detonation mode.

In the case of small $\varkappa$ (almost uniform heating of the gas) the reaction will run its course throughout the vessel and no shocks will form.

2. Equations and boundary conditions. The investigation of gas motion will begin with one-dimensional equations of gas dynamics, with the energy release resulting from the chemical reaction taken into consideration (a reaction of the first order with respect to a is taken for purposes of simplicity)

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho U}{\partial X}=0 \quad \left(\rho=\frac{1}{V}\right), \quad \frac{\partial U}{\partial t}+U\frac{\partial U}{\partial X}=-\frac{1}{\rho}\frac{\partial P}{\partial X}$$
$$\frac{\partial P}{\partial t}+U\frac{\partial P}{\partial X}+\gamma P\frac{\partial U}{\partial X}=(\gamma-1)Qapke^{-E/RT}, \quad \frac{\partial a}{\partial t}+$$
$$+U\frac{\partial a}{\partial X}=-kae^{-E/RT} \qquad (2.1)$$

Here Q is the energy release, E is the activation energy, k is a pre-exponential factor, and γ is the adiabatic exponent.

It will be convenient, for the subsequent investigation, to shift to the Lagrangian coordinate, x, and to dimensionless variables, through the following formulas

$$P = P_0 p, \quad T = T_0 \theta, \quad U = \sqrt{\gamma RT_0}\, u, \quad V = \frac{RT_0}{P_0} v$$
$$t = \frac{\tau}{k} \exp \frac{E}{RT_0}, \quad \varkappa = \frac{\lambda k T_0}{\sqrt{\gamma RT_0}} \exp\left(-\frac{E}{RT_0}\right)$$
$$x \frac{P_0 \sqrt{\gamma RT_0}}{kRT_0} \exp \frac{E}{RT_0} = \int_0^X \frac{dX}{V(t, X)} \qquad (2.2)$$
$$X = \xi \frac{\sqrt{\gamma RT_0}}{k} \exp \frac{E}{RT_0}$$

The equations of motion at (2.1) will take the form

$$\frac{1}{\gamma - 1} \frac{\partial \theta}{d\tau} + p \frac{\partial u}{\partial x} = \alpha a \exp\left[\beta\left(1 - \frac{1}{\theta}\right)\right], \quad \gamma \frac{\partial u}{\partial \tau} + \frac{\partial p}{\partial x} = 0 \qquad (2.3)$$
$$\frac{\partial a}{\partial \tau} + a \exp\left[\beta\left(1 - \frac{1}{\theta}\right)\right] = 0, \quad \frac{\partial \xi}{\partial \tau} = u, \quad \frac{\partial \xi}{\partial x} = v$$
$$\left(\alpha = \frac{Q}{RT_0}, \ \beta = \frac{E}{RT_0}\right)$$

Once Eq. (2.2) has been transformed, the original conditions, Eqs. (1.1) and (1.2), and the equation of state, Eq. (1.3), will be in the form /78

$$\theta(0, x) = e^{-\lambda x} \ (\theta(0, \xi) = 1 - \lambda\xi), \quad v(0, x) = \theta(0, x)$$
$$\xi(0, x) = \lambda^{-1}(1 - e^{-\lambda x}), \quad p(0, x) = 1, \quad a(0, x) = 1, \quad u(0, x) = 0, \qquad (2.4)$$
$$pv = \theta$$

Let us point out that if the function T(0, X) is extended evenly in the region $X < 0$, the statement of the problem can be considered a Cauchy problem.

3. The electronic computer computational scheme. The problem in the final section of the X axis must be considered in order to carry out the numerical integration of the system of Eq. (2.3) with original conditions

of Eq. (2.4). Let us introduce a wall with X = L. The boundary conditions (the condition for the impenetrability of walls) can be written

$$u(\tau, 0) = u(\tau, x^{(0)}) = 0 \qquad (3.1)$$
$$x^{(0)} = -\frac{1}{\lambda}\ln(1-\lambda\xi^{(0)}), \quad \xi^{(0)} = \frac{kL}{\sqrt{\gamma RT_0}}\exp\left(-\frac{E}{RT_0}\right)$$

The boundary condition at a cold wall here introduced and necessary in order to limit the region in which the equations are integrated, has no effect on the course of the reaction because we are interested in a period of time that is shorter than the period of time over which the forming shock wave reaches the right boundary.

The formation of shocks should be expected in the course of solving the problem, so, following Neuman and Richtmayer [1], let us introduce artificial viscosity in order to replace the shocks with a thin transition layer in which the magnitudes will change rapidly, but without a discontinuity. The introduction of artificial viscosity avoids the complex computation for shocks using Hugoniot equations. Artificial viscosity will be introduced through the following formula

$$q = \gamma\frac{(\nu\Delta x)^2}{v}\left(\frac{\partial u}{\partial x}\right)^2 \text{ при } \frac{\partial u}{\partial x} < 0;\ q = 0 \text{ при } \frac{\partial u}{\partial x} \geqslant 0 \qquad (3.2)$$

where Δx is a step along the space coordinate; ν is the coefficient of artificial viscosity.

And the first two expressions of Eq. (2.3) can be replaced by the equation

$$\frac{1}{\gamma-1}\frac{\partial\theta}{\partial\tau} + (p+q)\frac{\partial u}{\partial x} = \alpha\alpha\exp\left[\beta\left(1-\frac{1}{\theta}\right)\right]$$
$$\gamma\frac{\partial u}{\partial\tau} + \frac{\partial}{\partial x}(p+q) = 0 \qquad (3.3)$$

The following explicit algorithm for solving the problem is not difficult to obtain when the "tripod" type difference scheme [2] is taken

$$u_j^{n+1} = u_j^n - \frac{(\Delta\tau)_n}{\gamma\Delta x}\left(p_{j+1/2}^n + q_{j+1/2}^n - p_{j-1/2}^n - q_{j-1/2}^n\right)$$

$$\xi_j^{n+1} = \xi_j^n + (\Delta\tau)_n u_j^{n+1}, \quad v_j^{n+1} = (\Delta x)^{-1}\left(\xi_{j+1/2}^{n+1} - \xi_{j-1/2}^{n+1}\right)$$

$$a_j^{n+1} = a_j^n\left[1 + (\Delta\tau)_n f(\theta_j^n)\right]^{-1}, \quad f(\theta_j^n) = \exp\left[\beta\left(1 - \frac{1}{\theta_j^n}\right)\right]$$

$$p_j^{n+1} = \frac{(\gamma-1)^{-1}\theta_j^n + (1/2)p_j^n + q_j^n)(v_j^n - v_j^{n+1}) + \alpha(a_j^n - a_j^{n+1})}{1/2\left[(\gamma+1)(\gamma-1)^{-1}v_j^{n+1} - v_j^n\right]} \tag{3.4}$$

$$\theta_j^{n+1} = p_j^{n+1}v_j^{n+1}$$

$$q_j^n = \frac{2\gamma\nu^2}{v_j^n}\left(u_{j+1/2}^n - u_{j-1/2}^n\right)^2 \text{ при } u_{j+1/2}^n < u_{j+1/2}^n; \quad q_j^n = 0 \text{ при } u_{j+1/2}^n \geqslant u_{j-1/2}^n$$

$$0 \leqslant j \leqslant J \cdot (J\Delta x = x^{(0)}), \quad 0 \leqslant n < \infty$$

Here the value of the function φ at time $(\Delta\tau)_1 + (\Delta\tau)_2 + \ldots + (\Delta\tau)_n$ /79 at point in space $j\Delta x$ is designated by φ_j^n. The time step $(\Delta\tau)_n$ is selected on the basis of the Courant stability condition (it ensures that no increase will take place in the tiny errors that arise during the computation)

$$(\Delta\tau)_n = \frac{\Delta x\sqrt{\gamma/2\nu}}{\max_j\sqrt{\theta_j^n/v_j^n}} \tag{3.5}$$

The boundary and initial values of the magnitudes can be computed by using the following schemes:

(a) boundary conditions

$$u_0^{n+1} = \xi_0^{n+1} = u_J^{n+1} = q_0^{n+1} = q_J^{n+1} = 0, \quad \xi_J^n = \xi_0^{(0)}$$

$$a_J^n = a_J^{n-1}\left[1 + (\Delta\tau)_{n-1}f(\theta_J^{n-1})\right]^{-1}$$

$$a_0^n = a_0^{n-1}\left[1 + (\Delta\tau)_{n-1}f(\theta_0^{n-1})\right]^{-1}$$

$$v_J^n = v_J^{n-1} - \frac{(\Delta\tau)_{n-1}}{\Delta x}u_{J-1}^{n-1}, \quad p_J^n = \frac{\theta_J^n}{v_J^n}$$

$$v_0^n = v_0^{n-1} + \frac{(\Delta\tau)_{n-1}}{\Delta x}u_1^{n-1}, \quad p_0^n = \frac{\theta_0^n}{v_0^n} \tag{3.6}$$

$$\theta_J^n = \theta_J^{n-1} + (\Delta\tau)_{n-1}(\gamma-1)\alpha a_J^n f(\theta_J^{n-1}) + (\gamma-1)\frac{(\Delta\tau)_{n-1}}{\Delta x}u_{J-1}^{n-1}(p_J^{n-1} + q_J^{n-1})$$

$$\theta_0^n = \theta_0^{n-1} + (\Delta\tau)_{n-1}(\gamma-1)\alpha a_0^n f(\theta_0^{n-1}) - (\gamma-1)\frac{(\Delta\tau)_{n-1}}{\Delta x}u_0^{n-1}(p_0^{n-1} \pm q_0^{n-1})$$

(b) initial conditions

$$\theta_j^0 = \exp(-\lambda j/\Delta x), \quad \xi_j^0 = \lambda^{-1}\left[1 - \exp(-\lambda j/\Delta x)\right]$$
$$p_j^0 = a_j^0 = 1, \quad u_j^0 = 0, \quad v_j^0 = \theta_j^0 \tag{3.7}$$

4. Discussion of the results. The following values for the dimension-

less parameters included in the problem were selected for the computation: $v = 1.7$, $J = 350$, $\alpha = 5$, $\beta = 10$, $\gamma = 1.2$, $\xi^{(0)} = 55$.

Henceforth, the results will be illustrated in physical variables for $k = 10^{10}$ sec^{-1}, $T_o = 2000°K$ ($L = 10$ cm in this case).

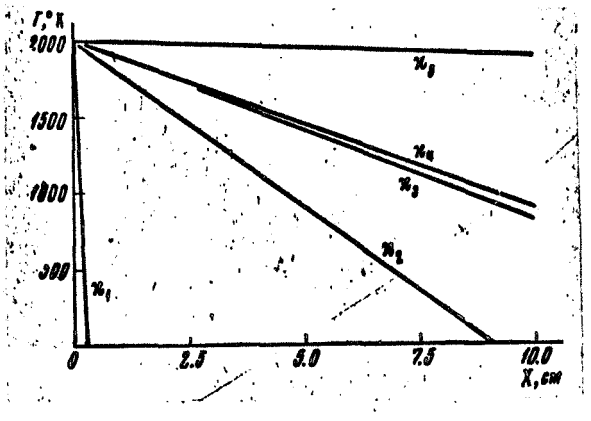


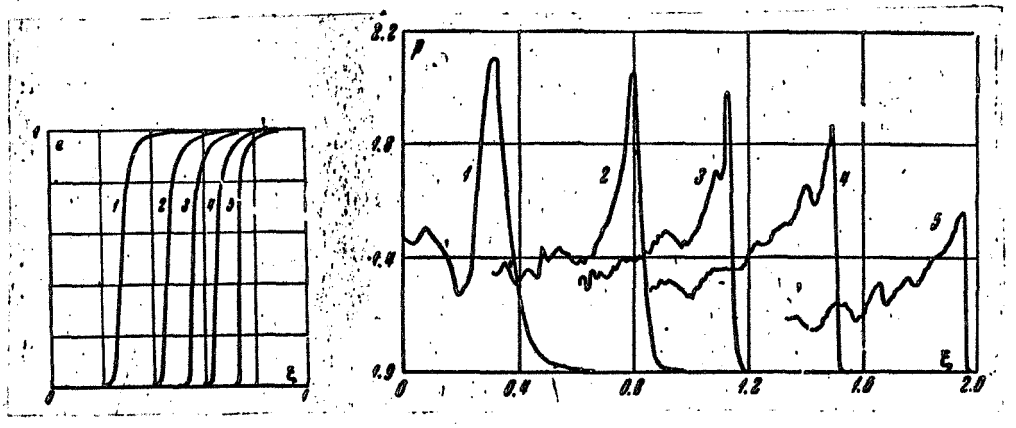
Figure 1

Moreover, we choose $\lambda_1 = 0.66$ ($\varkappa_1 = 7360$ °/cm), $\lambda_2 = 0.02$ ($\varkappa_2 = 220$), $\lambda_3 = 0.0107$ ($\varkappa_3 = 118$), $\lambda_4 = 0.01$ ($\varkappa_4 = 110$), $\lambda_5 = 0.001$ ($\varkappa_5 = 11$).

Figure 1 shows the initial temperature distribution for these $\varkappa$ values in physical variables.

First off, we will consider the case of large initial temperature gradients ($\lambda_1 = 0.66$). Figures 2 a, b, c and d show the distribution of the magnitudes a, p, θ and u with respect to the coordinate. Curves 1, 2, 3, 4, and 5 correspond to moments in time $\tau = 0.41$, 0.82, 1.22, 2.44, 3.93.

When $\tau \doteq 0.41$ the reaction wave and the shock wave coincide (Figure 2 a and b). At succeeding moments in time the distance between the shock wave and the reaction wave increases at an ever-increasing rate and the shock wave breaks away from the reaction wave.



Figures 2 a and b.

Figure 2b shows that the pressure behind the shock wave front pulsates, and that the pulsations with slight amplitude (ripples) can be separated

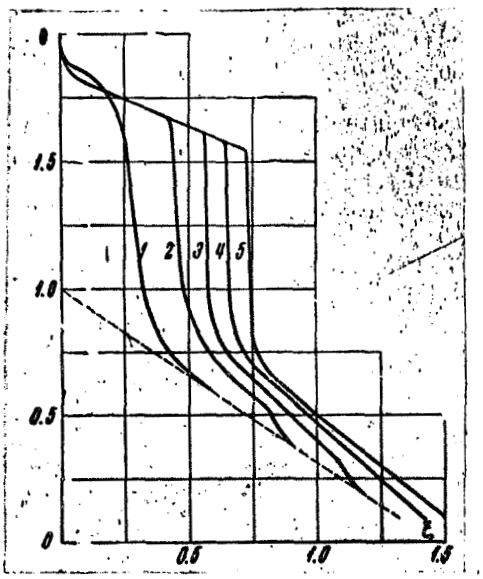


Figure 2c

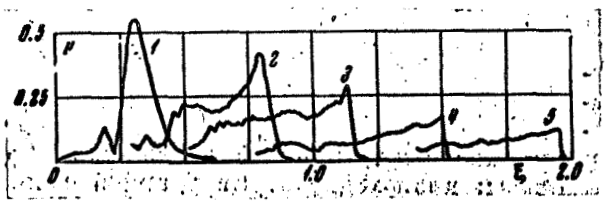


Figure 2d

from the large-scale pulsations that are acoustic disturbances propagating behind the shock wave front. The slight pressure oscillations in the wave profile are the result of the properties of the finite-difference scheme of Eq. (3.4). The magnitudes of these pulsations determine the accuracy with which the results obtained can be trusted. Maximum intensity of the shock wave is $p/p_o \cong 2.1$. After the shock wave breaks away from the reaction wave the shock wave is attenuated, with the result that the rarefaction wave (troughs in the wave profile) overtakes the shock wave.

The initial temperature distribution is shown by the dashed line in Figure 2c. As will be seen, a basic increase in the temperature will induce a reaction wave. Heating of the gas by the shock wave is slight. The reaction wave therefore slows (Figure 2a).

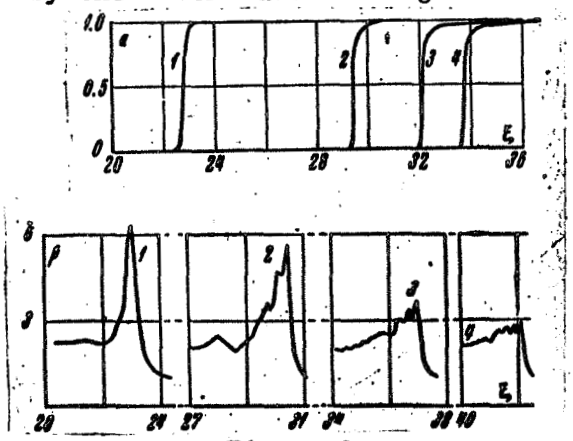


Figure 3

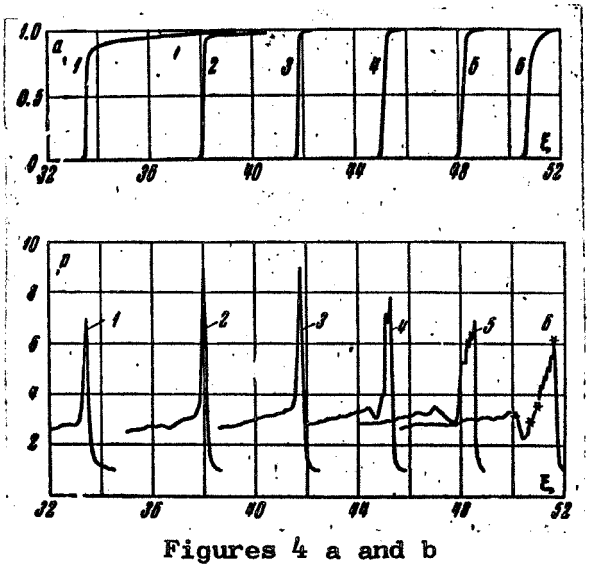
If the equations contained terms describing the diffusion and thermal conductivity, what would be formed would be a normally propagating flame. Let us point out that the velocity of flame propagation, so the absence of these terms has no effect on the formation and propagation of the shock wave.

Figure 2d shows the change in gas velocity over time with respect to the walls.

The same reaction condition can be realized for $\lambda_2 = 0.02$. Figure 3 /81

shows the distribution of the magnitudes a and p. Curves 1, 2, 3 and 4 correspond to the time values τ = 7.44, 11.49, 16.65, 22.15.

The difference between this case and the preceding one is that the shock wave breaks away from the reaction wave much later in time and at greater distances from the hot wall (when τ = 7.44 and ξ = 23.0 they still coincide), because a large mass of reacting gas takes part in the formation of the shock wave. This is why the maximum intensity of the shock wave is considerably greater than in the preceding case, and is equal to 6.6.



Figures 4 a and b

Figures 4 a and b show the course of the reaction in the detonation mode. Here λ_3 = 0.0107. This is that critical gradient, λ_1^*, at which detonation occurs. Corresponding to curves 1, 2, 3, 4, 5 and 6, obtained as a result of the solution, are time values τ = 5.73, 7.84, 9.53, 11.23, 12.96, 14.76. Wave velocity can be computed from Figure 4, and equals 15.07, 5.57, 5.80, 5.29, 4.88, 4.53 at the above-indicated time intervals (the magnitude of the velocity has been reduced to the speed of sound at 300°K).

On the other hand, from the formula for a heavy detonation [3]

$$D = \sqrt{2(\gamma^2 - 1)Q} \qquad (4.1)$$

where D is the detonation wave velocity, we obtain D = 4.95.

As will be seen, at time τ = 14.76, the detonation wave enters the Chapman-Jouguet mode. This can be confirmed by computing the detonation wave velocity with respect to the products of the detonation, which latter is equal to the local speed of sound. The computations were made at the points marked by the asterisks in Figure 4b. The magnitude (D-w)/c (w is the velocity of the reaction products at the particular point; c is the speed of sound at this same point) equals 0.97, 1.06, 0.98, 0.53 (in ascending

order of ξ). The latter magnitude equates to the point where the reaction has not yet begun. The deviations from unity of the magnitudes cited are within the limits of accuracy for the determination of wave velocity.

The disparity between the wave velocities computed as a result of the computation, and as a result of using Eq.(4.1), can be explained, it would appear, by the fact that the structure of a detonation wave is nonstationary. /82 This has been pointed out in [4-6], in which the unstable nature of one-dimensional propagation of a detonation wave was investigated. We too observed the pressure pulsations at the wave front noted in [5,6] (the results will not be included here). We should point out that in [5,6], as distinguished from the case under consideration, the velocity of the detonation wave, and the degree of supercompression, were fixed by external conditions, that is, by piston movement.

It should also be recalled that the very consideration of a plane detonation wave is quite conditional because of its instability in the face of spatial deformations. The detonation waves observed experimentally have a complex, three-dimensional, nonstationary structure. Hence, the computation made in the foregoing can but illustrate the first stage in the formation of a detonation wave that has not yet succeeded in forming its spatial structure.

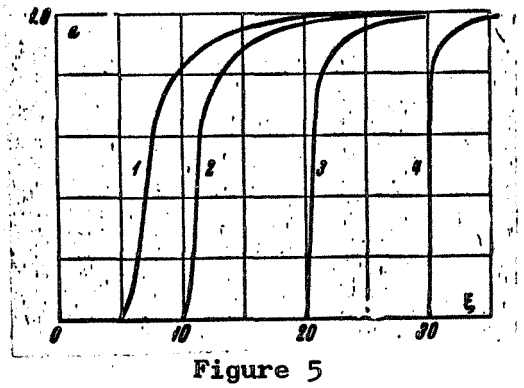


Figure 5

Let us make a comparison between /83 the results obtained and the propagation of the reaction in an incompressible gas. Setting the derivative $\partial u/\partial x = 0$ in Eq. (2.3), it is easy to obtain the following relationship determining the change in concentration, a, over time

$$e^{\beta\tau} = Ei\left[\frac{\beta}{\Delta - a\sigma}\right] - Ei\left[\frac{\beta}{\Delta - \sigma}\right] + e^{\beta/\Delta}\left\{Ei\left[\frac{\beta\sigma}{\Delta(\Delta-\sigma)}\right] - Ei\left[\frac{\beta a\sigma}{\Delta(\Delta - a\sigma)}\right]\right\} \qquad (4.2)$$

$$\left(\sigma = a(\gamma - 1),\ \Delta = 1 + \sigma - \lambda\xi,\ Ei[x] = \int_{-\infty}^{x} \frac{e^z\,dz}{z},\ x > 0\right)$$

The results of the computations made in arriving at the solutions of

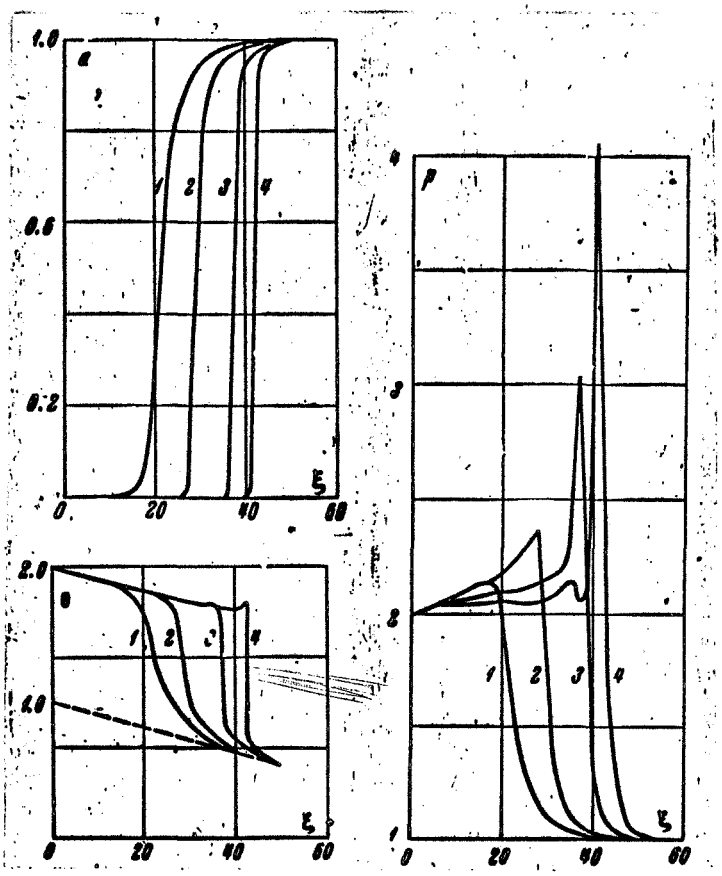


Figure 6

Eq. (4.2) are shown in Figure 5, where curves 1, 2, 3 and 4 correspond to moments in time τ = 0.27, 0.42, 1.34, 6.75 (λ_3 = 0.0107)

Figures 6 a, b and c enable us to follow the formation of the detonation wave (λ_4 = 0.01). The solutions for 1, 2, 3 and 4 correspond to moments in time τ = 1.55, 3.10, 7.75, 10.75. The initial distribution of all magnitudes is quite flat, but then, because of the formation of the wave, the gradient becomes increasingly steeper. Here the wave is formed later than in the preceding case.

If now there is an even greater reduction in the slope of the temperature profile, beginning at λ_2^* = 0.003, the reaction takes place throughout the vessel; that is we have a thermal explosion mode.

Let us point out that the values of the critical gradients λ_1^* and λ_2^* are functions of vessel length. In fact, if the length of the vessel is less than the distance over which the Chapman-Jouguet mode is arrived at,

the mode in which the reaction occurs can be classified as a thermal explosion.

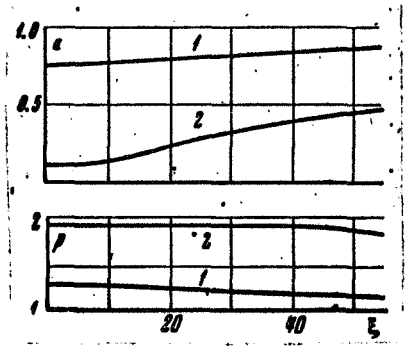


Figure 7

Figure 7 shows the solution of $\lambda_5 = 0.001$, with curves 1 and 2 plotted for $\tau = 0.18$ and 0.34. Complete burn-out of the combustible component occurs at $\tau = 0.47$. Pressure throughout the vessel is raised almost uniformly at $2P_o$. This is readily obtainable from the system of Eq. (2.1) if the x derivatives are set equal to zero.

5. An explanation of the nature of knocking in internal combustion engines. The process involved in burning up the fuel mixture in internal combustion engines can be accompanied by an explosion. This phenomenon has come to be called knocking. Today it is accepted that this phenomenon can be explained from the point of view of kinetic concepts. At the same time, the conclusions arrived at by the various authors are extremely contradictory and do not provide anywhere near the explanations that should be available from accumulated experimental material. Monographs [7,8] contain detailed discussions of existing views on this question. We should also point out reference [9], a recent paper.

The purely thermal explanation of this phenomenon suggested in our paper is based on the possibility of the occurrence of a detonation wave as a result of the nonuniform heating of the reaction-capable gas mixture. The formation of the detonation wave can explain the reason why high thermal and mechanical overloading of the engine can be observed during knocking. For example, when $\lambda_3 = 0.0107$, the intensity of the forming detonation wave is equal to ~ 6. In accordance with the formula for the reflection of a detonation wave from a solid wall [10], the pressure beyond the reflected wave is equal to $\sim 15P_o$.

The formation of detonation waves during knocking were observed in the experiments. They are described in [8].

The authors wish to express their deep appreciation to L. A. Chudov for his great help in solving the problem. /84

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